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SOME ASYMPTOTIC FORMULAS FOR MARKOV CHAINS WITH  
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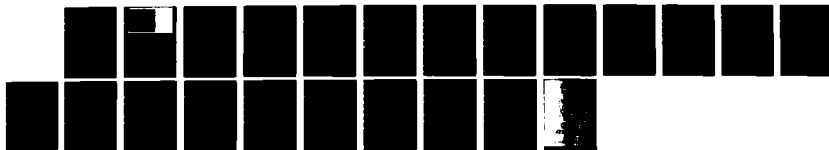
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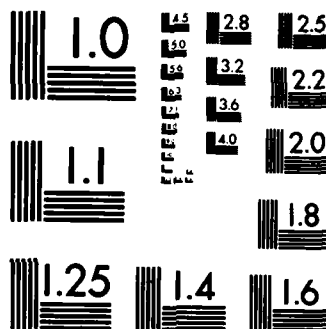
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SOME ASYMPTOTIC FORMULAS FOR MARKOV  
CHAINS WITH APPLICATIONS TO SIMULATION

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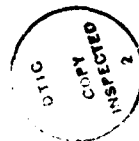
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ABSTRACT

Formulas are derived for the initial bias, variance, and spectrum of the sample mean in finite state Markov processes. The focus is on application of such expressions to the steady-state simulation problem.

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## SIGNIFICANCE AND EXPLANATION

Various techniques have been proposed for determination of confidence intervals associated with steady-state quantities in simulation. Evaluation of such procedures requires comparison of their performance on stochastic systems with known characteristics. In this paper, we therefore derive <sup>the initial</sup> computable formulas for several quantities associated with finite state Markov chains, and discuss their relevance to the steady-state simulation problem.

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The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the author of this report.

SOME ASYMPTOTIC FORMULAS FOR MARKOV CHAINS  
WITH APPLICATIONS TO SIMULATION

Peter W. Glynn

1. INTRODUCTION

Consider the simulation of a stochastic process  $\{X_t : t \geq 0\}$  for which

$$(1.1) \quad X_t \Rightarrow X$$

( $\Rightarrow$  denotes weak convergence). In many simulation applications, it is of interest to determine confidence intervals for  $r(f) \triangleq Ef(X)$ , where  $f$  is some real-valued functional defined on the state space of  $X_t$ . This problem is known, in the simulation literature, as the steady-state simulation problem, and a great deal of effort has been devoted toward its solution; see Chapter 5 of Fishman (1978) or Section 8.6 of Law and Kelton (1982) for a complete discussion of the problem.

The evaluation of simulation methodology for the steady-state simulation problem requires that one possess a class of models for which parameters of interest may be calculated analytically. Behavior of the procedures on the models then provides a "benchmark" from which to judge their overall performance. Our goal, in this paper, is to establish a variety of formulas for finite state Markov chains (in both discrete and continuous time) and to discuss the importance of these formulas in the context of methodology evaluation.

One of the earliest techniques proposed for dealing with steady-state simulation problems is the technique of replication. The simulator chooses  $t$  large, and simulates the process up to time  $t$ , creating a sample path  $\{x_s^1 : 0 \leq s \leq t\}$ . The simulator repeats this step  $m$  times, creating a collection  $\{x_s^i : 0 \leq s \leq t\}$ ,  $1 \leq i \leq m$ , of  $m$  independent replicates of the process. The parameter  $r(f)$  is then estimated by

$$r_t(m, f) = \frac{1}{mt} \sum_{i=1}^m \int_0^t f(x_s^i) ds.$$

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Note that the independence of the replicates yields a central limit theorem, and a consequent asymptotically valid confidence interval. In any case, the mean square error of the estimate  $r_t(m, f)$  is given by

$$(1.2) \quad E(r_t(m, f) - r(f))^2 = \sigma^2(r_t(1, f))/m + b_t^2(f)$$

where

$$b_t(f) = E r_t(1, f) - r(f) .$$

It is clear that for large  $m$ , the bias term  $b_t(f)$  is the primary contributor to the mean square error. As a result, the initial bias term  $b_t(f)$  has attracted a great deal of attention in the simulation literature; for a survey, see Wilson and Pritsker (1978). Section 2 is therefore devoted to formulas for  $b_t(f)$ , and to a qualitative discussion of initial bias.

More recently, a variety of single replicate procedures have been proposed. They rely on the fact that for many processes  $X_t$  satisfying (1.1), there exists a constant  $s(f)$ , depending on the process  $X_t$ , such that

$$(1.3) \quad \sqrt{t} \left( \int_0^t f(X_s) ds / t - r(f) \right) / s(f) \Rightarrow N(0, 1)$$

where  $N(0, 1)$  is a unit normal random variable (result (1.3) holds, in particular, for finite state Markov chains). Confidence intervals based on (1.3) require consistent estimators for the constant  $s^2(f)$ . In Section 3, formulas are derived for the constant  $s^2(f)$ , thereby allowing the study and comparison of different estimators for  $s^2(f)$ . These formulas extend the work of Hazen and Pritsker (1980) on continuous time Markov chains with diagonalizable generators to the general case. Section 4 is devoted to solution of several related conjectures of Hazen and Pritsker.

One well-studied class of estimators for  $s^2(f)$  is based on spectral techniques. If  $\{X_t\}$  is a second order stationary process, it can be shown, under certain regularity conditions, that  $s^2(f) = 2\pi c(0)$ , where  $c(\lambda)$  is the spectrum of  $\{X_t\}$  given by

$$(1.4) \quad c(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\lambda t} \text{cov}(f(X_0), f(X_t)) dt .$$

Several recent papers (see Heidelberger and Welch (1981a), (1981b), for example) have proposed techniques based on estimating  $s^2(f)$  via polynomial fitting to an estimated spectrum in a neighborhood of zero. Section 5 therefore derives formulas for the spectrum corresponding to finite state Markov chains.

Before concluding this section, it should be noted that the above discussion for continuous time processes carries over, in an obvious way, to discrete time processes - this justifies the interest in formulas for discrete time Markov chains.



## 2. FORMULAS FOR THE INITIAL BIAS

Let  $\{X_n : n \geq 0\}$  be an irreducible Markov chain of period  $d$ , with transition matrix  $P$ , on state space  $E = \{1, 2, \dots, m\}$ . Such a chain necessarily has a unique stationary distribution  $\pi = (\pi_1, \dots, \pi_m)$  solving  $\pi P = \pi$ . Given a row vector  $f' = (f(1), \dots, f(m))$  ( $f'$  denotes the transpose of  $f$ ), it is well known that

$$\frac{1}{n} \sum_{k=0}^{n-1} f(X_k) \rightarrow \pi f$$

with probability 1, for any initial distribution  $\mu = (\mu_1, \dots, \mu_m)$  ( $\mu_i = P\{X_0 = i\}$ ). Let

$$b_n(\mu, f) = E_{\mu} \left( \frac{1}{n} \sum_{k=0}^{n-1} f(X_k) \right) - \pi f ;$$

here  $E_{\mu}(\cdot)$  stands for expectation under initial distribution  $\mu$ . Our objective is to obtain formulas for the initial bias  $b_n(\mu, f)$ .

We will need the following standard results from Markov chain theory (see Kemeny and Snell (1960), p. 70, 71, 100):

$$(2.1) \quad P^{nd} \rightarrow \Pi_0 \text{ as } n \rightarrow \infty, \text{ where } \Pi_0 \text{ is a stochastic matrix}$$

$$(2.2) \quad \Pi = (I + P + \dots + P^{d-1})/d, \text{ where } \Pi \text{ has all rows equal to } \pi$$

$$(2.3) \quad P\Pi = \Pi = \Pi^2 = \Pi$$

$$(2.4) \quad \text{the inverse matrix } \hat{F} = (\Pi - \hat{Q})^{-1} \text{ exists, where } \hat{Q} = P - I.$$

The matrix  $\hat{F}$  is called the fundamental matrix of the Markov chain. It is worth noting that when  $P$  is aperiodic, the matrix  $\hat{F}$  has the representation  $\hat{F} = \sum_{k=0}^{\infty} (P - \Pi)^k$ . Since the natural analog of  $\Pi$  for transient chains is the zero matrix, it follows that the fundamental matrix is a generalized form of the potential matrix (see Cinlar (1975), p. 196-7).

(2.5) Theorem. The initial bias  $b_n(\mu, f)$  is given by

$$(2.6) \quad b_n(\mu, f) = \mu(I - P^n)\hat{F}f/n.$$

Furthermore, if  $n = kd + i$ , where  $0 \leq i < d$ , then

$$(2.7) \quad b_n(\mu, f) = \mu(I - P^i\Pi_0)\hat{F}f/n + o(p^n)$$

where  $0 < p < 1$  (a sequence  $b_n$  is  $o(a_n)$  if there exists  $K > 0$  such that

$$|b_n| < K|a_n|).$$

Proof. The bias can be written in the form

$$b_n(\mu, f) = \frac{1}{n} \sum_{k=0}^{n-1} \sum_{i,j} \mu_i p_{ij}^k f(j) - \sum_{i,j} \mu_i \pi_j f(j) = \frac{1}{n} \sum_{k=0}^{n-1} \mu(P^k - \Pi) f.$$

Now, it is easily verified, using (2.3), that

$$(2.8) \quad \sum_{k=0}^{n-1} (P^k - \Pi)(\Pi - \hat{Q}) = I - P^n$$

from which (2.6) follows immediately, after postmultiplying through (2.8) by  $\hat{F}$ . Equation (2.7) is a direct consequence of the geometric convergence of  $P^{nd}$  to  $\Pi_0$  (see Corollary 4.1.5 of Kemeny and Snell (1960)). ||

This result generalizes Theorem 7-15 of Heyman and Sobel (1982) (their proof requires that  $P$  be aperiodic). We now illustrate the application of the theorem to a two state Markov chain. Let

$$P = \begin{pmatrix} 1-a & a \\ b & 1-b \end{pmatrix}$$

where  $a, b > 0$  and  $0 < a + b < 2$ . Then  $\{X_n\}$  is aperiodic and

$$\pi = \frac{1}{a+b} (b \quad a)$$

with

$$\hat{F} = \frac{1}{a+b} \begin{pmatrix} b & a \\ b & a \end{pmatrix} + \frac{1}{(a+b)^2} \begin{pmatrix} a & -a \\ -b & b \end{pmatrix}.$$

Hence

$$b_n(\mu, f) = \frac{1}{(a+b)^2 n} (a\mu_1 - b\mu_2)(f(1) - f(2)) + o(\rho^n).$$

A similar bias formula can be obtained for continuous time Markov chains. Let  $\{X_t : t > 0\}$  be an irreducible Markov jump process on state space  $E = \{1, 2, \dots, m\}$ , with generator  $Q$  (recall that  $Q$  generates  $X_t$  in the sense that  $P(t) = \exp(Qt)$ , where  $P_{ij}(t) = P(X_t = j | X_0 = i)$ ) and unique stationary distribution  $\pi$  solving  $\pi Q = 0$ . Retaining the notational conventions previously stated, set

$$b_t(\mu, f) = E_\mu \left( \frac{1}{t} \int_0^t f(X_s) ds \right) - \pi f.$$

The following results are well known:

$$(2.9) \quad P(t) \rightarrow \Pi, \text{ where } \Pi \text{ has all rows identical to } \pi$$

$$(2.10) \quad P(t)\Pi = \Pi P(t) = \Pi^2 = \Pi.$$

We will also need the following lemma.

$$(2.11) \quad \text{Lemma. The inverse matrix } F = (\Pi - Q)^{-1} \text{ exists.}$$

Proof. Using (2.10) and the fact that  $\Pi Q = 0 = Q\Pi$ , observe that

$$(2.12) \quad (\Pi - Q) \left( \int_0^t (P(s) - \Pi) ds + \Pi \right) = - \int_0^t Q \exp(Qs) ds + \Pi = I - \exp(Qt) + \Pi.$$

Then, letting  $\|A\| = \max_i \left\{ \sum_j |A_{ij}| \right\}$ , we have

$$\int_0^\infty \|P(s) - \Pi\| ds = \sum_{n=0}^\infty \int_0^1 \|P(n) - \Pi\| P(s) ds < \sum_{n=0}^\infty \|P(n) - \Pi\|$$

which is finite, since  $P(1)$  is an aperiodic irreducible matrix and therefore  $P(n)$  converges to  $\Pi$  geometrically fast. Hence, letting  $t \rightarrow \infty$  in (2.12), we see that  $\Pi - Q$  has an inverse. ||

Initial bias for continuous time Markov chains is determined by the following theorem.

$$(2.13) \quad \text{Theorem. The bias } b_t(\mu, f) \text{ is given by}$$

$$b_t(\mu, f) = \mu(I - P(t))Ff/t = \mu(I - \Pi)Ff/t + o(e^{-\alpha t}),$$

where  $\alpha$  is some positive constant.

The proof of this theorem is similar to that given in the discrete time case. It should be pointed out that Theorem 2.13 generalizes a result of Grassman (1982) given for  $f(k) = k$ .

These initial bias formulas have several interesting properties. First of all, we observe that there exists a constant  $c(\mu, f)$  such that

$$t^k (b_t(\mu, f) - c(\mu, f)/t) \rightarrow 0$$

for all  $k > 0$ . Hence, in any bias expansion of the form

$$b_t(\mu, f) = \sum_{k=1}^K c_k(\mu, f)/t^k + o(t^{-K-1}),$$

it must be that  $c_i(\mu, f) = 0$  for  $i > 2$ . Secondly, for any  $\mu$  and  $f$ , there exists  $t$  such that for  $s > t$ , either:

- i)  $b_s(\mu, f)$  decreases monotonically to zero, or
- ii)  $b_s(\mu, f)$  increases monotonically to zero.

Hence, for  $s$  sufficiently large, the bias has a constant sign. Several proposed initial bias procedures require this sign consistency property (see, for example, Schruben (1982), p. 577). Of course, the above discussion is equally valid for discrete time chains (provided one accounts for periodicity).

### 3. VARIANCE FORMULAS FOR THE SAMPLE MEAN

A natural way to try to evaluate  $s(f)$  is to take the variance of both sides of (1.3), yielding the formal relation

$$(3.1) \quad t \sigma^2 \left( \int_0^t f(X_s) ds / t \right) \rightarrow s^2(f) .$$

For finite state Markov chains, relation (3.1) can be justified rigorously, in the sense that it is correct that

$$(3.2) \quad t E_{\pi} \left( \frac{1}{t} \int_0^t f(X_s) ds - \pi f \right)^2 \rightarrow s^2(f) ,$$

a similar result holds in discrete time. For continuous time Markov chains, (3.2) can be proved by using the fact that  $\{X_t : t \geq 0\}$  is  $\phi$ -mixing and then applying Theorem 20.1 of Billingsley (1968). The discrete time version of (3.2) follows from Theorem 3 of Chung (1966), p. 102. The following theorem therefore provides a formula for evaluation of  $s^2(f)$ .

(3.3) Theorem. Let  $\{X_n : n \geq 0\}$  and  $\{X_t : t \geq 0\}$  satisfy the same assumptions as in Section 2. Then,

$$(3.4) \quad n E_{\pi} \left( \frac{1}{n} \sum_{k=0}^{n-1} f(X_k) - \pi f \right)^2 = f' T (I - P) f + 2 f' T P (P - I) f + \frac{2}{n} f' T (P^{n+1} - P) P^2 f$$

$$(3.5) \quad t E_{\pi} \left( \frac{1}{t} \int_0^t f(X_s) ds - \pi f \right)^2 = 2 f' T (P - I) f + \frac{2}{t} f' T (P(t) - I) P^2 f ,$$

where  $T$  is a diagonal matrix with  $T_{ii} = \pi_i$ .

Proof. The process  $\{X_n\}$  is stationary under  $P_{\pi}(\cdot)$ , so

$$(3.6) \quad n E_{\pi} \left( \frac{1}{n} \sum_{k=0}^{n-1} f(X_k) - \pi f \right)^2 = \text{var}_{\pi} f(X_0) + \frac{2}{n} \sum_{k=1}^{n-1} (n-k) \text{cov}_{\pi}(f(X_0), f(X_k)) .$$

Now,

$$(3.7) \quad \text{cov}_{\pi}(f(X_0), f(X_k)) = \sum_{i,j} \pi_i f(i) P_{ij}^k f(j) - \sum_{i,j} \pi_i \pi_j f(i) f(j) = f' T(P^k - \Pi) f$$

and

$$(3.8) \quad \sum_{k=1}^{n-1} (n-k)(P^k - \Pi)(\Pi - \hat{Q}) = \sum_{k=1}^{n-1} (n-k)(P^k - P^{k+1})$$

$$= nP - \sum_{k=1}^n P^k = n(P - \Pi) - \sum_{k=0}^n (P^k - \Pi) + I - \Pi.$$

Applying (2.8) to the sum in (3.8), and postmultiplying through (3.8) by  $\hat{F}$  yields

$$(3.9) \quad \sum_{k=1}^{n-1} (n-k)(P^k - \Pi) = n(P - \Pi)\hat{F} - (I - P^{n+1})\hat{F}^2 + (I - \Pi)\hat{F}.$$

Since  $\Pi(\Pi - \hat{Q}) = \Pi$ , it follows that  $\Pi = \Pi\hat{F}$ . Also,  $\hat{Q} = (\Pi - I)(\Pi - \hat{Q})$  so that  $\hat{Q}\hat{F} = \Pi - I$  and thus  $\hat{Q}\hat{F}^2 = (\Pi - I)\hat{F}$ . These observations, together with (3.6), (3.7), and (3.9), lead directly to (3.4). The proof of (3.5) is similar. ||

The right hand side of (3.5) can be algebraically rearranged, by using the identity  $F - \Pi = \Pi - (\Pi + Q)^{-1}$ , to obtain Theorem 1 of Hazen and Pritsker (1980). Their derivation required, however, that  $Q$  be diagonalizable. The formula also extends equation (16) of Grassman (1982) to general  $f$ . Formula (3.4) is an exact form of an asymptotic result found on page 84 of Kemeny and Snell (1960).

We now apply Theorem 3.3 to determine  $s^2(f)$  for the two state Markov chain studied in Section 2. Routine calculations show that

$$s^2(f) = f' T(I - \Pi) f + 2f' T P(\hat{F} - \Pi) f = \frac{ab(2 - a - b)}{(a + b)^3} (f(1) - f(2))^2.$$

We can, in fact, extend Theorem 3.3 to cover arbitrary initial distributions.

(3.10) Theorem. Let  $\{X_n : n \geq 0\}$  and  $\{X_t : t \geq 0\}$  satisfy the same assumptions as in Section 2. Then,

$$n \mathbb{E}_{\mu} \left( \frac{1}{n} \sum_{k=0}^{n-1} f(X_k) - \pi f \right)^2 = s^2(f) + o\left(\frac{1}{n}\right)$$

$$t \mathbb{E}_{\mu} \left( \frac{1}{t} \int_0^t f(X_s) ds - \pi f \right)^2 = s^2(f) + o\left(\frac{1}{t}\right).$$

**Proof.** We prove only the case where  $\{X_n\}$  is aperiodic; the periodic and continuous time proofs require only simple modification. Let  $g(j) = f(j) - \pi f$  and observe that

$$\begin{aligned} (3.11) \quad n \left| \mathbb{E}_{\mu} \left( \frac{1}{n} \sum_{k=0}^{n-1} g(X_k) \right)^2 - \mathbb{E}_{\pi} \left( \frac{1}{n} \sum_{k=0}^{n-1} g(X_k) \right)^2 \right| \\ = \left| \frac{1}{n} \sum_{k=0}^{n-1} \mathbb{E}_{\mu} g^2(X_k) - \mathbb{E}_{\pi} g^2(X_0) + \frac{2}{n} \sum_{k=0}^{n-2} \sum_{l=k+1}^{n-1} (\mathbb{E}_{\mu} g(X_k)g(X_l) - \mathbb{E}_{\pi} g(X_k)g(X_l)) \right|. \end{aligned}$$

Now,  $P^n \rightarrow \Pi$  geometrically fast (see Corollary 4.1.5 of Kemeny and Snell (1960)) so there exist constants  $\alpha > 0$  and  $0 < \rho < 1$  such that  $|P_{ij}^k - \pi_j| < \alpha \rho^k$ . Thus, for  $l > k$ ,

$$\begin{aligned} |\mathbb{E}_{\mu} g(X_k)g(X_l) - \mathbb{E}_{\pi} g(X_k)g(X_l)| &= \left| \sum_{i,j} \mu_i g(i) (P_{ij}^k - \pi_j) \sum_r (P_{jr}^{l-k} - \pi_r) g(r) \right| \\ &< |g|^2 \sum_{i,j,r} \mu_i \alpha^2 \rho^l = |g|^2 \pi \alpha^2 \rho^l \end{aligned}$$

where  $|g| = \max_i |g(i)|$ . This inequality, together with Theorem 2.5, allows one to bound

(3.11) by

$$|b_n(\mu, g^2)| + \frac{2}{n} |g|^2 \pi \sum_{k=0}^{n-2} \sum_{l=k+1}^{n-1} \alpha^2 \rho^l = o(1/n).$$

Application of (3.4) completes the proof. ||

Theorem 3.10 allows us to obtain an asymptotic formula for the mean square error of the estimator  $r_t(m, f)$  used in the method of replication. By (1.2), and Theorems 2.5, 3.3, and 3.10,

$$\begin{aligned}
E_{\mu}(x_t(m, f) - \pi f)^2 &= E_{\mu}(x_t(m, g))^2 = \frac{1}{m} (E_{\mu}(x_t(1, g))^2 - E_{\mu}^2 x_t(1, g)) + b_t^2(\mu, g) \\
&= \frac{2}{mt} f' T(F - \Pi) f + \frac{1}{t^2} (\mu(I - \Pi) F f)^2 + o\left(\frac{1}{mt}\right),
\end{aligned}$$

an analogous expansion holds in the discrete time setting.



#### 4. SOLUTION TO CONJECTURES OF HAZEN AND PRITSKER

In their study of continuous time Markov chains, Hazen and Pritsker considered the dependence of  $s(f)$  on scaling of the generator  $Q$ . Writing  $s(Q, f)$  to indicate the dependence of  $s(f)$  on  $Q$ , they showed that if  $\alpha > 0$ , then  $s^2(\alpha Q, f) = s^2(Q, f)/\alpha$  for finite state processes and conjectured that the same result holds for countable state processes, as well. The following theorem answers their conjecture (see Feller (1971), p. 326-32 for definitions and results on Markov jump processes).

(4.1) Theorem. Let  $Q$  be an irreducible conservative (i.e.  $Q_{ij} > 0$  for  $i \neq j$ ,  $-\infty < Q_{ii} = -\sum_j Q_{ij}$ ) generator. If the minimal process  $\{X_t\}$  corresponding to  $Q$  satisfies

$$P_\mu \left\{ \left( \int_0^t (f(X_s) - r(f)) ds \right) < x\sqrt{t} s(Q, f) \right\} \rightarrow P\{N(0, 1) < x\}$$

as  $t \rightarrow \infty$ , then the minimal process  $\{\hat{X}_t\}$  corresponding to  $\alpha Q$ , for  $\alpha > 0$ , satisfies

$$P_\mu \left\{ \left( \int_0^t (f(\hat{X}_s) - r(f)) ds \right) < x\sqrt{t} s(\alpha Q, f) \right\} \rightarrow P\{N(0, 1) < x\}$$

and  $s^2(\alpha Q, f) = s^2(Q, f)/\alpha$ .

Proof. Since  $\{X_t\}$  is the minimal process corresponding to  $Q$ , it follows that it may be constructed via a discrete time Markov chain  $\{Y_k\}$  that determines the sequence of states visited by  $X_t$ , with the holding time in the  $k^{\text{th}}$  state visited given by an exponential random variable with parameter  $q(Y_k)$  ( $q(i) = -Q_{ii}$ ). On the other hand, the minimal process  $\hat{X}_t$  associated with  $\alpha Q$  has the same embedded discrete time chain  $\{Y_k\}$ , but with holding times determined by exponential random variables with parameters  $\alpha q(Y_k)$ . Hence, one can represent  $\hat{X}_t$  via  $\hat{X}_t = X_{\alpha t}$ , so that

$$\begin{aligned} \left( \int_0^{\alpha t} (f(X_s) - r(f)) ds \right) / t^{1/2} \alpha^{1/2} &= \left( \int_0^{\alpha t} (f(\hat{X}_{s/\alpha}) - r(f)) ds \right) / t^{1/2} \alpha^{1/2} \\ &= \alpha^{1/2} \left( \int_0^t (f(\hat{X}_s) - r(f)) ds \right) / t^{1/2}, \end{aligned}$$

from which the theorem follows. ||

An application of the result shows that the variance constant  $s^2(Q, f)$  for the queue-length process associated with an M/M/1 queue with arrival rate  $\alpha\lambda$  and service rate  $\alpha\mu$  is proportional to  $1/\alpha$  (see p. 31 of Hazen and Pritsker (1980)).

Before proceeding to the second conjecture of Hazen and Pritsker, it is convenient to discuss a second group of formulas for  $s^2(f)$ , based on the regenerative structure of finite state Markov chains. The regenerative property dictates that blocking the sample path of the process according to consecutive entrance times  $T_j$  into some fixed state, say  $i$ , yields a sequence of independent and identically distributed random variables. It is to be expected, then, that the variance constant  $s^2(f)$  can be evaluated in terms of quantities expressed over a single regenerative block. In fact, it can be shown that (see Smith (1955), Theorem 9)

$$(4.2) \quad s^2(f) = E_1 \left( \int_0^{T_1} (f(X_s) - \bar{f}) ds \right)^2 / E_1 T_1$$

where  $E_1(\cdot)$  denotes the expectation conditional on  $X_0 = i$  (a similar formula holds in discrete time; see Chung (1966), p. 99). Hordijk, Iglehart, and Schassberger (1976) derive matrix-theoretic expressions for the numerator and denominator of (4.2). From a historical viewpoint, it is interesting to note that there is a third group of formulas for  $s^2(f)$ , based on the eigenstructure of the transition matrices; see Romanovsky (1970), p. 241.

Returning now to the second conjecture, consider a capacity one single server queue with Poisson arrivals and Erlang- $p$  service times, with inter-arrival and service time means given by  $1/\lambda$  and  $p/\mu$  respectively. If one is interested in the variance constant associated with the number of customers in queue, then the method of stages shows that the constant may be evaluated by considering  $s^2(f)$  for the continuous time Markov chain described by the  $(p+1)$  by  $(p+1)$  generator

$$Q = \begin{pmatrix} -\lambda & 0 & 0 & \dots & \lambda \\ \mu & -\mu & 0 & \dots & 0 \\ 0 & \mu & -\mu & \dots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & \mu & -\mu \end{pmatrix}$$

where  $f = (0, 1, 1, \dots, 1)$  (i.e.  $f$  is one so long as the customer is in service). Writing  $s^2(p, \mu, f)$  to denote the dependence of  $s^2(f)$  on  $p$  and  $\mu$ , the conjecture of Hazen and Pritsker was that for  $\mu > 0$ ,

$$(4.3) \quad s^2(p, p\mu, f) = \frac{p+1}{2p} s^2(1, \mu, f) .$$

Relation (4.3) can be most easily proved by using (4.2). Let  $Z_0, Z_1, \dots, Z_p$  be independent exponential random variables with  $EZ_0 = 1/\lambda$  and  $EZ_i = 1/p\mu$  for  $i > 1$ . Then,

$$(4.4) \quad E_1 T_1 = E(Z_0 + \dots + Z_p) = 1/\lambda + 1/\mu$$

$$(4.5) \quad E_1 \left( \int_0^{T_1} (f(X_s) - \pi f) ds \right)^2 = E_1 \left( -\pi f Z_0 + \sum_{i=1}^p Z_i (1 - \pi f) \right)^2$$

$$= (\pi f)^2 \frac{1}{\lambda^2} + (1 - \pi f)^2 \frac{1}{p\mu^2} = \frac{1}{(\lambda + \mu)^2} \left( \frac{p+1}{p} \right) ,$$

since  $\pi f = \lambda/(\lambda + \mu)$ . Substituting (4.4) and (4.5) into (4.2), one gets

$$s^2(p, p\mu, f) = \left( \frac{p+1}{p} \right) \frac{\lambda\mu}{(\lambda + \mu)^3} ,$$

verifying (4.3). Incidentally, it is easily shown, using (4.2), that  $s^2(p, p\mu, f)$  tends to the variance constant associated with the constant service time version of the model as  $p \rightarrow \infty$ , as would be expected.

## 5. FORMULAS FOR THE SPECTRAL DENSITY

The spectral density of a discrete time Markov chain is defined by

$$\hat{c}(\lambda) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} e^{i\lambda k} \text{cov}_\pi(f(X_0), f(X_k)) ;$$

for continuous time Markov chains,  $c(\lambda)$  is given by

$$c(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\lambda t} \text{cov}_\pi(f(X_0), f(X_t)) dt .$$

The spectral density of finite state Markov chains may be computed via the following theorem.

(5.1) Theorem. Let  $\{X_n\}$  and  $\{X_t\}$  satisfy the same assumptions as in Section 2. Then, the inverse matrices  $\hat{P}(\lambda) = (\Pi - \hat{Q} + (e^{i\lambda} - 1)I)^{-1}$  and  $P(\lambda) = (\Pi - Q + i\lambda I)^{-1}$  exist for all  $\lambda$ , and the spectral densities  $\hat{c}(\lambda)$  and  $c(\lambda)$  are given by

$$(5.2) \quad 2\pi \hat{c}(\lambda) = f'T(I - \Pi)f + f'TP(\hat{P}(-\lambda) + \hat{P}(\lambda) - \Pi(e^{i\lambda} + e^{-i\lambda}))f$$

$$(5.3) \quad 2\pi c(\lambda) = f'T(P(-\lambda) + P(\lambda) - 2\Pi/(1 + \lambda^2))f$$

Proof. We give the proof in the discrete time aperiodic case, the proofs in the other cases being similar. Using (3.7), one gets

$$(5.4) \quad 2\pi \hat{c}(\lambda) = f'T(I - \Pi)f + \sum_{k=1}^{\infty} (e^{-i\lambda k} + e^{i\lambda k}) f'T(P^k - \Pi)f .$$

Now, observe that

$$(5.5) \quad \sum_{k=1}^n e^{i\lambda k} (P^k - \Pi)(\Pi - P + e^{-i\lambda} I) = P - \Pi - e^{i\lambda n} (P^{n+1} - \Pi) .$$

Also, it is evident that

$$\sum_{k=1}^{\infty} |e^{i\lambda k} (P^k - \Pi)| < \sum_{k=1}^{\infty} |P^k - \Pi| < \infty$$

since  $P^k \rightarrow \Pi$  geometrically fast, and thus the sum in (5.5) converges to some limit, say  $D(\lambda)$ . Taking limits in (5.5) yields

$$D(\lambda)(\Pi - P + e^{-i\lambda} I) = P - \Pi$$

so

$$e^{i\lambda}(D(\lambda) + I)(\Pi - P + e^{-i\lambda}I) = I$$

and thus  $\hat{F}(-\lambda) = (\Pi - \hat{Q} + (e^{-i\lambda} - 1)I)^{-1}$  exists. Postmultiplying through (5.5) by  $\hat{F}(-\lambda)$  and letting  $n \rightarrow \infty$  proves that

$$(5.6) \quad \sum_{k=1}^{\infty} e^{i\lambda k} (P^k - \Pi) = (P - \Pi)\hat{F}(-\lambda).$$

It is easily verified that  $\Pi\hat{F}(\lambda) = e^{i\lambda}\Pi$  and combination of (5.4) and (5.6) leads easily to (5.2). ||

Formulas (5.2) and (5.3), together with Theorem 3.3, prove that  $2\pi c(0) = s^2(f)$  (see (1.4)), justifying the use of spectral methods for finite state Markov chains. Returning to the two state Markov chain introduced earlier, the computation of  $\hat{c}(\lambda)$  is straightforward, given that

$$\begin{aligned} \hat{F}(\lambda) &= \frac{1}{e^{i\lambda}(b+a-1) + e^{i2\lambda}} \begin{pmatrix} b & a \\ b & a \end{pmatrix} \\ &+ \frac{1}{(e^{i\lambda}(b+a-1) + e^{i2\lambda})(a+b)} \begin{pmatrix} e^{i\lambda}(a+b) - b & -a \\ -b & e^{i\lambda}(a+b) - a \end{pmatrix} \end{aligned}$$

The formulas also yield some interesting qualitative information about the spectrum of finite state Markov chains. Applying Cramer's rule to compute the inverse matrix  $\hat{F}(\lambda)$  shows that the elements of  $\hat{F}(\lambda)$  are always rational polynomials in the indeterminate  $e^{i\lambda}$  - in fact, the polynomials describing the numerator and denominator must be of degree less than or equal to  $m$ . Consequently, the spectrum of a stationary discrete time finite state Markov chain corresponds to that of a finite order autoregressive moving average process.

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